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Generation of high-fidelity controlled-not logic gates by coupled superconducting qubits

Andrei Galiautdinov

Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602, U.S.A.

ag@physast.uga.edu

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Abstract

Building on the previous results of the Weyl chamber steering method, we demonstrate how to generate high-fidelity controlled-not by direct application of certain, physically relevant Hamiltonians with *fixed coupling constants* containing Rabi terms. Such Hamiltonians are often used to describe two superconducting qubits driven by local *rf*-pulses.

It is found that in order to achieve 100% fidelity in a system with *capacitive* coupling of strength g one Rabi term suffices. We give the exact values of the physical parameters needed to implement such CNOT. The gate time and all possible Rabi frequencies are found to be $t = \pi/(2g)$ and $\Omega_1/g = \sqrt{64n^2 - 1}$, $n = 1, 2, 3, \ldots$. Generation of a perfect CNOT in a system with *inductive* coupling, characterized by additional constant k, requires the presence of both Rabi terms. The gate time is again $t = \pi/(2g)$, but now there is an infinite number of solutions, each of which is valid in a certain range of k and is characterized by a pair of positive integers (n, m),

$$\frac{\Omega_{1,2}}{g} = \sqrt{16n^2 - \left(\frac{k-1}{2}\right)^2} \pm \sqrt{16m^2 - \left(\frac{k+1}{2}\right)^2}.$$

We distinguish two cases, depending on the sign of the coupling constant: (1) the *antiferromagnetic* case ($k \geq 0$) with $n \geq m = 0, 1, 2, \ldots$; (2) the *ferromagnetic* case ($k \leq 0$) with $n > m = 0, 1, 2, \ldots$.

The paper concludes with consideration of fidelity degradation by switching to resonance. Simulation of time-evolution based on the 4th order Magnus expansion reveals characteristics of the gate similar to those found in the exact case, with slightly shorter gate time and shifted values of Rabi frequencies.

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1 Introduction

The goal of this paper is to show how to successfully generate, with a minimal amount of effort, a high-fidelity CNOT in systems consisting of coupled superconducting qubits described by Hamiltonians with *coupling constants fixed by architecture*. We want to find out if making a CNOT in such systems can, at least theoretically, be reduced to a simple push of a button. Once initially set, the system itself would then take care of the needed gate by freely evolving from the identity of the unitary group to the target along the corresponding geodesic.

We thus approach the subject of time-control from the "opposite", non-optimal end. The plug-and-play implementations considered in this paper may be useful for simple gate designs which do not rely on sophisticated time-control of their physical parameters. The question of simplicity will also become important once the best qubit is identified, and put together with thousands of others to form an integrated circuit. Optimally controlling [1] qubits in such a circuit would become a difficult task, potentially leading to a compromise between the optimal and the simple. Thus, in this paper we limit our attention mostly to time-independent Hamiltonians. The only place where time dependence necessarily arises is in the analysis of fidelity degradation due to switching to resonance, considered in Section 6.

Two important developments motivated our work. The first was a series of experiments [2, 3, 4] which showed that the macroscopic quantum states [5, 6] of Josephson junctions have coherence times long enough for such states to be used as qubits. That led to our choice of the physical Hamiltonians. The other development was the work on the Weyl chamber steering method [7, 8] in which several examples of direct generation of various important gates, including CNOT, was considered from a purely geometrical standpoint.

In what follows we will use the square brackets $[\cdots]$ to denote the gate — a representative of a given local class — located in a Weyl chamber.

2 The concept of local equivalence

We begin by recalling the notion of local equivalence within the special unitary group $SU(4)$. Two gates $U_1, V_1 \in SU(4)$ are *locally equivalent* if they differ only by local transformations:

$$U_1 \sim V_1 \Longleftrightarrow U_1 = k_1\, V_1\, k_2, \quad k_1, k_2 \in SU(2) \otimes SU(2). \tag{1}$$

It is obvious that local equivalence is an example of equivalence relation: it is reflexive ($U \sim U$), symmetric ($U \sim V \Longleftrightarrow V \sim U$), and transitive ($U \sim V,\ V \sim W \Longrightarrow U \sim W$). When an equivalence relation is given on a set, it partitions the set into disjoint classes. Thus the entire group $SU(4)$ is partitioned into classes of locally equivalent elements; any such element (a two qubit gate) belongs to one and only one local equivalence class.

To generalize the concept of local equivalence to the full $U(4)$ we use the fact that any $U \in U(4)$ can be written in the form $U = e^{i\,\alpha}\, U_1$, with $U_1 \in SU(4)$ (even though, as groups, $U(4) \neq U(1) \otimes SU(4)$). Then two gates $U = e^{i\,\alpha}\, U_1, V = e^{i\,\beta}\, V_1 \in U(4)$ are locally equivalent if their representatives in $SU(4)$ are equivalent:

$$U \sim V \Longleftrightarrow U_1 \sim V_1. \tag{2}$$

One way to represent local classes in $SU(4)$ is with the help of a Cartan decomposition of the underlying Lie algebra $L = su(4)$. This can be seen as follows:

For any *semi-simple* Lie algebra L, its Cartan decomposition is a direct sum of two *subspaces* $L = K \oplus P$, one of which, K, is itself a Lie algebra, $[K, K] \subset K$, and the other, P, satisfies

$[P,\,P] \subset K$, $[P,\,K] \subset P$. Because $K \cap P = 0$, any subalgebra $A \subset P$ must necessarily be abelian. Such *maximal* abelian subalgebra $A_C \subset P$ is called the Cartan subalgebra of L relative to the given Cartan decomposition. An important Cartan decomposition theorem (for *groups*) states that if a semisimple algebra L has decomposition $L = K \oplus P$, then any element $U_1 \in \exp L$ can always be written in the form

$$U_1 = k_1\, V_1\, k_2, \tag{3}$$

where $V_1 \in \exp A_C$, and $k_1, k_2 \in \exp K$.

An example of a Cartan decomposition is provided by $su(2)$, for which we can take $K = \mathrm{span}\{\frac{i}{2}\sigma_z\}$, $P = \mathrm{span}\{\frac{i}{2}\sigma_x,\ \frac{i}{2}\sigma_y\}$, and $A_C = \mathrm{span}\{\frac{i}{2}\sigma_x\}$.

Cartan decompositions of $su(4)$ are more complicated, but a special choice [1] of K spanned by the local operators

$$X_1 = \frac{i}{2}\sigma_x^1,\quad Y_1 = \frac{i}{2}\sigma_y^1,\quad Z_1 = \frac{i}{2}\sigma_z^1,\quad X_2 = \frac{i}{2}\sigma_x^2,\quad Y_2 = \frac{i}{2}\sigma_y^2,\quad Z_2 = \frac{i}{2}\sigma_z^2, \tag{4}$$

and P spanned by all nonlocal operators $\frac{i}{2}\,\sigma_\alpha^1\sigma_\beta^2$ $(\alpha, \beta = x, y, z)$ is particularly useful. If we now take the span of mutually commuting operators

$$XX = \frac{i}{2}\,\sigma_x^1\sigma_x^2,\quad YY = \frac{i}{2}\,\sigma_y^1\sigma_y^2,\quad ZZ = \frac{i}{2}\,\sigma_z^1\sigma_z^2 \tag{5}$$

to serve as A_C, the Cartan decomposition theorem applied to $SU(4) = \exp[su(4)]$ gives

$$U_1 = k_1\,\exp\left(c_1 XX + c_2 YY + c_3 ZZ\right) k_2. \tag{6}$$

This results in a convenient representation of $SU(4)$ local equivalence classes by the *class vectors* $[c_1, c_2, c_3] \in A_C$. Representation of the $U(4)$ classes is up-to-phase the same,

$$U = e^{i\,\alpha}\, k_1\,\exp\left(c_1 XX + c_2 YY + c_3 ZZ\right)\, k_2. \tag{7}$$

The correspondence between class vectors and equivalence classes is *not* one-to-one: there are certain symmetries which map class vectors to other class vectors of the same equivalence class. However it was shown in [7] that the correspondence can be made unique by restricting class vectors to a tetrahedral region in A_C, called a Weyl chamber. One such chamber, denoted by a^+, is chosen to be canonical — it is described by the following three conditions [7, 9]:

- $\pi > c_1 \geq c_2 \geq c_3 \geq 0$,
- $c_1 + c_2 \leq \pi$,
- if $c_3 = 0$, then $c_1 \leq \pi/2$.

Even though the choice of the Weyl chamber is not unique, when fixed, it becomes a powerful tool for analyzing time evolution on the full $U(4)$.

In the original papers on the subject [7, 8], several implementations of various useful gates by steering on a^+ have been demonstrated. Of particular interest to us is the way $[\mathrm{CNOT}] = [\pi/2, 0, 0] \in a^+$ was generated by a *single* application of Hamiltonians with *controllable* Ising type interaction, such as

$$H_{yy} = \Omega_{1x}\sigma_x^1 + \Omega_{2x}\sigma_x^2 + \Omega_{1z}\sigma_z^1 + \Omega_{2z}\sigma_z^2 + g\sigma_y^1\sigma_y^2, \tag{8}$$

and similarly for H_{xx}, H_{zz}. In [7, 8], the local invariants of the corresponding unitary evolution $U(t) = \exp(iH_{yy}t)$ were first found in closed analytic form. Numerical analysis then produced the values for the time and the coupling constants needed to achieve a perfect [CNOT] in just one application. The

yy and zz cases are particularly interesting because their interaction parts (when viewed as elements of A_C) point in the direction "perpendicular" to [CNOT].

Let us now turn to Hamiltonians used to describe coupled superconducting qubits. Such Hamiltonians may contain several Ising terms, which we choose to be fixed by architecture (*cf.* [10, 11]). Our goal is to find out if they are also capable of generating [CNOT] in a single application, and if so, how many Rabi terms are required in order for such generation to be successful.

3 Hamiltonians for coupled superconducting qubits

When restricted to the two-qubit subspace, the Hamiltonian for two capacitively coupled phase qubits driven by *rf*-pulses is given by

$$H_{\text{fast}} = \underbrace{-\sum_{i=1}^{2} \frac{\omega_i}{2} \sigma_z^i}_{H_0} + \underbrace{\sum_{i=1}^{2} \Omega_i \cos(\omega_{\text{rf}}^i t + \delta_i)\sigma_x^i + g\sigma_y^1 \sigma_y^2}_{V}, \quad g > 0. \tag{9}$$

The level spacings ω_i are tunable between about 7 to 10 GHz. The Rabi frequencies Ω_i and the phases δ_i are fully controllable.

As it stands, this Hamiltonian is not suitable for actual gate implementations because of the very small time scale ($t_{\text{sc}} \sim 0.1$ ns) associated with ω_i. The scale roughly corresponds to the time it takes to make a "round trip" on $SU(4)$ when going in the direction of $-iH \in su(4)$. To attain high fidelity of the gate we would have to control the pulses with accuracy which is experimentally unattainable.

To avoid this problem, the rotating wave approximation (RWA) is used. We set the frequency of the external pulse to be equal to the transition frequency of the system (resonance), $\omega_{\text{rf}}^i = \omega_i \equiv \omega$, bring the phases to zero, and work in the interaction picture, in which the time evolution is governed by

$$\begin{aligned} H &= e^{iH_0 t} V e^{-iH_0 t} \\ &= \sum_{i=1}^{2} \Omega_i \left[\cos^2(\omega t)\sigma_x^i + \frac{\sin(2\omega t)}{2}\sigma_y^i\right] + g\left[\cos(\omega t)\sigma_y^1 - \sin(\omega t)\sigma_x^1\right]\left[\cos(\omega t)\sigma_y^2 - \sin(\omega t)\sigma_x^2\right]. \end{aligned} \tag{10}$$

After averaging over fast oscillations the Hamiltonian becomes

$$H = \frac{\Omega_1}{2}\sigma_x^1 + \frac{\Omega_2}{2}\sigma_x^2 + \frac{g}{2}\left(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2\right), \tag{11}$$

or in the language of Lie algebra $su(4)$,

$$-iHt = -t\left[\Omega_1 X_1 + \Omega_2 X_2 + g\,(XX + YY)\right]. \tag{12}$$

There is an interesting modification of this qubit architecture based on inductive coupling between the qubits (see Appendix). In that case an additional coupling constant k is introduced resulting in the full Hamiltonian

$$-iHt = -t\left[\Omega_1 X_1 + \Omega_2 X_2 + g\,(XX + YY + kZZ)\right]. \tag{13}$$

4 Implementing [CNOT] by time-independent Hamiltonians

4.1 The $XX + YY$ case

Here we show how to implement the perfect [CNOT] by a single application of the experimentally available Hamiltonian (12) with one Rabi term

$$-\,iHt = -t\,\left[\Omega_1\,X_1 + g\,(XX + YY)\right]\ . \tag{14}$$

We first establish a useful group-theoretical result about the exponentials of (14). We consider a subalgebra of $su(4)$, $A_0 = \mathrm{span}\{X_1, XX, YY, ZY\}$, whose generators obey the commutation relations summarized in the following table:

$$A_0 : \quad \begin{array}{|c|cccc|} \hline & X_1 & XX & YY & ZY \\ \hline X_1 & 0 & 0 & -ZY & YY \\ XX & 0 & 0 & 0 & 0 \\ YY & ZY & 0 & 0 & -X_1 \\ ZY & -YY & 0 & X_1 & 0 \\ \hline \end{array} \quad . \tag{15}$$

Notice that ZY generator had to be added to the set of generators in order to ensure closure under commutation.

The generator XX is central in A_0. Its span is a one-dimensional abelian ideal $I \subset A_0$, which makes A_0 into a *non*-semisimple Lie algebra. This algebra is a direct sum of two subspaces, $A_0 = I \oplus A_1$, with $A_1 = \mathrm{span}\{X_1, YY, ZY\}$ *isomorphic* to $su(2)$.

Exponentiation of A_0 results in a *four*-dimensional subgroup $G_0 = \exp A_0 \subset SU(4)$ whose every element W can be written as a product

$$W = e^{-c_1\,XX}\,\underbrace{e^{-a\,X_1 - c_2\,YY - b\,ZY}}_{\text{an element of }\ \exp A_1}. \tag{16}$$

Because A_1 has its own Cartan decomposition (*e.g.*, $A_1 = \mathrm{span}\{X_1\} \oplus \mathrm{span}\{YY, ZY\}$ with Cartan subalgebra $A_C = \mathrm{span}\{YY\}$), application of the Cartan decomposition theorem to the group $G_1 = \exp A_1$ gives

$$W = e^{-c_1\,XX}\,e^{-\alpha\,X_1}\,e^{-c_2\,YY}\,e^{-\beta\,X_1}. \tag{17}$$

Now, because $e^{-iHt} = e^{-t[\Omega_1 X_1 + g(XX+YY)]}$ is itself an element of $G_0 = \exp A_0$, it can also be written as such product

$$e^{-t[\Omega_1 X_1 + g(XX+YY)]} = e^{-\alpha\,X_1}\,e^{-c_1\,XX - c_2\,YY}\,e^{-\beta\,X_1}\,, \tag{18}$$

where the commutativity of X_1 and XX has been used to rearrange the factors on the right.

Thus given any gate (t, Ω_1, g) generated by H in (14), with coupling g fixed by architecture, there always exists a set of four numbers $(\alpha,\ c_1,\ c_2,\ \beta)$ which represent that gate exactly. This is essentially the same good old Cartan decomposition theorem (6) for $SU(4)$, restricted to a physically relevant subgroup G_0 associated with experimentally available Hamiltonian (14).

By fixing Ω_1 and evolving the system freely under the action of its Hamiltonian, we generate a flow along a straight line in $su(4)$ which has its image in both, the Weyl chamber and the group $SU(4)$.

The converse is unfortunately not necessarily true: for a given gate $(\alpha,\ c_1,\ c_2,\ \beta)$ it is not always possible to find (t, Ω_1) generating that gate. This is because of noncommutativity between X_1 and YY.

Even though there is no guarantee that H would be able to reach every $(c_1, c_2, 0)$ equivalence class in a single application, it is interesting to find out what actually *can* be reached. In particular, we want to know if [CNOT] is reachable.

It is obvious that if $\Omega_1 = 0$, then any local class with $c_1 = c_2$ and $c_3 = 0$ can be directly reached. What if $\Omega_1 \neq 0$?

We will be interested in purely geodesic solutions to (18). Thus, setting $\alpha = \beta = 0$ and directly exponentiating in (18) we get the matrix equation

$$\begin{bmatrix} \cos b_1 - \cos a & 0 & icd \sin a & i(\sin b_1 - d \sin a) \\ 0 & \cos b_2 - \cos a & i(\sin b_2 + d \sin a) & icd \sin a \\ icd \sin a & i(\sin b_2 + d \sin a) & \cos b_2 - \cos a & 0 \\ i(\sin b_1 - d \sin a) & icd \sin a & 0 & \cos b_1 - \cos a \end{bmatrix} = 0, \tag{19}$$

where

$$a = \frac{tg}{2} \sqrt{1 + \left(\frac{\Omega_1}{g}\right)^2}, \quad b_{1,2} = \frac{1}{2}(tg - c_1 \pm c_2), \quad c = \frac{\Omega_1}{g}, \quad d = \frac{1}{\sqrt{1 + \left(\frac{\Omega_1}{g}\right)^2}}. \tag{20}$$

If $\Omega_1 \neq 0$, then $\sin a = 0$, leading to $\cos a = \pm 1$ and $\cos b_1 = \cos b_2 = \pm 1$, $\sin b_{1,2} = 0$. This is only possible if $b_1 = b_2 + 2\pi m$, or

$$c_2 = 2\pi m, \quad m = 0, 1, 2, \ldots. \tag{21}$$

The minimal time solution is therefore

$$\begin{aligned} t_{\min} &= \frac{c_1}{g}, \\ \frac{\Omega_1}{g} &= \sqrt{\left(\frac{4\pi n}{c_1}\right)^2 - 1}, \quad n = 1, 2, 3, \ldots. \end{aligned} \tag{22}$$

Thus, by following H along its geodesic for a time $t_{\min}$ we can (exactly) reach any equivalence class located on the XX axis of the Weyl chamber. It is clear that the coupling constant g plays the role of the scaling factor between the coordinate c_1 of the point on this axis and the actual, *physical* time required to reach that point.

We want to emphasize that the corresponding trajectory in the Weyl chamber is *not* a straight line from O to [CNOT], even though is is a straight line in the full Lie algebra $su(4)$. This is because with Ω_1 now being fixed by (22), it is not true that $e^{-t[\Omega_1 X_1 + g(XX+YY)]} \sim e^{-c_1(t)\, XX}$ is satisfied for all intermediate times $0 < t < t_{\min}$. In general for such times, $c_2(t) \neq 0$ in (18).

One important local class belonging to the XX axis is [CNOT], which can be made by exponentiating the Hamiltonian $-iH_{[\mathrm{CNOT}]}t = -tXX$ with $t = \pi/2$. The corresponding matrix in the computational basis is

$$[\mathrm{CNOT}] = \exp\left(-\frac{\pi}{2} XX\right) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ -i & 0 & 0 & 1 \end{bmatrix} \in SU(4). \tag{23}$$

The Makhlin invariants [12] of this [CNOT] are $G_1 = 0$ and $G_2 = 1$, as required, so this is a perfectly acceptable [CNOT] out of which the canonical CNOT with matrix

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \in U(4) \tag{24}$$

can be produced by local manipulation of individual qubits. We will give some examples of the needed for this local *rf*-pulses in Section 5.

Thus, setting $c_1 = \pi/2$ in (22), we get

$$\begin{aligned} t_{\min} &= \pi/(2g), \\ \Omega_1/g &= \sqrt{64n^2-1}, \quad n = 1,2,3,\dots\ . \end{aligned} \tag{25}$$

The simplest exact [CNOT] is then

$$[\mathrm{CNOT}] = e^{-\frac{\pi}{2g}\,[\sqrt{63}gX_1 + g(XX+YY)]}\ . \tag{26}$$

For completeness we mention another [CNOT] solution to (18),

$$\Omega_1/g = \sqrt{16n^2-1}, \quad n = 1,2,3,\dots\ , \tag{27}$$

which is *up-to-phase* geodesic,

$$[\mathrm{CNOT}] = e^{2\pi\,X_1} e^{-\frac{\pi}{2g}\,[\Omega_1 X_1 + g(XX+YY)]}\ . \tag{28}$$

4.2 The $XX + YY + kZZ$ case

We are now going to show that a single application of the Hamiltonian given in (13) generates the exact [CNOT], provided both Rabi terms are kept.

Derivation parallels the previous case. We concentrate on subalgebra $A_0 \subset su(4)$:

$$A_0 : \quad \begin{array}{|c|ccccccc|} \hline & X_1 & X_2 & XX & YY & ZZ & YZ & ZY \\ \hline X_1 & 0 & 0 & 0 & -ZY & YZ & -ZZ & YY \\ X_2 & 0 & 0 & 0 & -YZ & ZY & YY & -ZZ \\ XX & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ YY & ZY & YZ & 0 & 0 & 0 & -X_2 & -X_1 \\ ZZ & -YZ & -ZY & 0 & 0 & 0 & X_1 & X_2 \\ YZ & ZZ & -YY & 0 & X_1 & -X_1 & 0 & 0 \\ ZY & -YY & ZZ & 0 & X_1 & -X_2 & 0 & 0 \\ \hline \end{array}\ . \tag{29}$$

The generator XX is again central in A_0, spanning a one-dimensional abelian ideal $I \subset A_0$. This makes A_0 into a non-semisimple Lie algebra which is a direct sum of two subspaces, $A_0 = I \oplus A_1$, where $A_1 = \mathrm{span}\{X_1, X_2, YY, ZZ, YZ, ZY\}$.

Exponentiation of A_0 results in a *seven*-dimensional subgroup $G_0 = \exp A_0 \subset SU(4)$ whose every element W can be written as a product

$$W = e^{-c_1\,XX}\,\underbrace{e^{-a\,X_1 - b\,X_2 - c_2\,YY - c_3\,ZZ - d\,YZ - f\,ZY}}_{\text{an element of }\exp A_1}. \tag{30}$$

Because A_1 has its own Cartan decomposition (*e.g.*, $A_1 = \mathrm{span}\{X_1, X_2\} \oplus \mathrm{span}\{YY, ZZ, YZ, ZY\}$ with a Cartan subalgebra $A_C = \mathrm{span}\{YY, ZZ\}$), application of the Cartan decomposition theorem to the group $G_1 = \exp A_1$ gives

$$W = e^{-c_1\,XX}\,e^{-\alpha\,X_1 - \beta\,X_2}\,e^{-c_2\,YY - c_3\,ZZ}\,e^{-\eta\,X_1 - \xi\,X_2}. \tag{31}$$

Since $e^{-iHt} = e^{-t[\Omega_1 X_1 + \Omega_2 X_2 - g(XX+YY+kZZ)]}$ is itself an element of $G_0 = \exp A_0$, it can also be written as such product

$$e^{-t[\Omega_1 X_1 + \Omega_2 X_2 + g(XX+YY+kZZ)]} = e^{-\alpha X_1 - \beta X_2}\, e^{-c_1 XX - c_2 YY - c_3 ZZ}\, e^{-\eta X_1 - \xi X_2}. \tag{32}$$

Thus, given any gate $(t, \Omega_1, \Omega_2, g, k)$ generated by H in (13), with couplings g and k fixed by architecture, there always exists a set of seven numbers (α, β, c_1, c_2, c_3, η, ξ) which represent that gate exactly. This is again the Cartan decomposition theorem for $SU(4)$, this time restricted to a physically relevant subgroup G_0 associated with experimentally available Hamiltonian (13).

With $\alpha = \beta = \eta = \xi = 0$, equation (32) has an infinite number of minimal time solutions labelled by pairs of integers (n, m) and valid in certain intervals of k,

$$\begin{aligned} t_{\min} &= \frac{c_1}{g}, \\ \frac{\Omega_{1,2}}{g} &= \sqrt{\left(\frac{2\pi n}{c_1}\right)^2 - \left(\frac{k-1}{2}\right)^2} \pm \sqrt{\left(\frac{2\pi m}{c_1}\right)^2 - \left(\frac{k+1}{2}\right)^2}. \end{aligned} \tag{33}$$

For [CNOT], $(c_1, c_2, c_3) = (\pi/2, 0, 0)$, which gives

$$\begin{aligned} t_{\min} &= \pi/2g, \\ \frac{\Omega_{1,2}}{g} &= \sqrt{16n^2 - \left(\frac{k-1}{2}\right)^2} \pm \sqrt{16m^2 - \left(\frac{k+1}{2}\right)^2}. \end{aligned} \tag{34}$$

Two cases will be distinguished here, depending on the sign of the coupling constant.

4.2.1 kZZ coupling of antiferromagnetic type

In this case, $k \geq 0$ and $n \geq m = 0, 1, 2, 3, \ldots$. The previous result for $k = 0$ is correctly recovered when $n = m = 0$. For $n = m = 1, 2, \ldots$ we get an (n, n)-th solution valid in the interval $0 \leq k \leq 8n - 1$.

Below, we list Rabi frequencies required to generate a *perfect plug-and-play* [CNOT] in the antiferromagnetic case for several values of n and m:

k	$\Omega_1^{(1,1)}/g$	$\Omega_2^{(1,1)}/g$	$\Omega_1^{(2,1)}/g$	$\Omega_2^{(2,1)}/g$	$\Omega_1^{(2,2)}/g$	$\Omega_2^{(2,2)}/g$	$\Omega_1^{(3,3)}/g$	$\Omega_2^{(3,3)}/g$
0.00	7.937254	0.000000	11.952987	4.015733	15.968719	0.000000	23.979157	0.000000
0.10	7.936614	0.012600	11.949341	4.025327	15.968405	0.006262	23.978949	0.004170
0.25	7.933253	0.031513	11.942076	4.040336	15.966755	0.015658	23.977852	0.010426
0.50	7.921238	0.063121	11.925151	4.067034	15.960859	0.031327	23.973935	0.020856
1.00	7.872983	0.127017	11.872983	4.127017	15.937254	0.062746	23.958261	0.041739
3.00	7.337085	0.408882	11.401356	4.473152	15.683221	0.191287	23.790420	0.126101
5.00	6.109853	0.818350	10.391718	5.100215	15.162165	0.329768	23.451110	0.213209
7.00	2.645751	2.645751	7.416198	7.416198	14.344402	0.487995	22.932659	0.305242
9.00					13.173201	0.683205	22.222421	0.404996
11.00					11.536501	0.953495	21.301017	0.516407
13.00					9.164486	1.418519	20.139099	0.645511
15.00					3.872983	3.872983	18.691066	0.802522
17.00							16.881526	1.007018
19.00							14.570504	1.304004
21.00							11.429081	1.837418
23.00							4.795832	4.795832

(35)

Notice that the product of Rabi frequencies for solutions of (n, n)-type is always equal to k,

$$\Omega_1^{(n,n)} \Omega_2^{(n,n)} / g^2 = k. \tag{36}$$

4.2.2 kZZ coupling of ferromagnetic type

In this case, $k \leq 0$ and $n > m = 0, 1, 2, \ldots$. A particularly interesting family of solutions occurs for $m = 0$. These solutions (*cf.* (27)) exist only for the coupling constant $k = -1$:

$$\Omega_{1,2}^{(n,0)} / g = \sqrt{16n^2 - 1}, \quad n = 1, 2, 3, \ldots. \tag{37}$$

For certain $n > m = 1, 2, 3$ we find:

k	$\Omega_1^{(2,1)}/g$	$\Omega_2^{(2,1)}/g$	$\Omega_1^{(3,1)}/g$	$\Omega_2^{(3,1)}/g$	$\Omega_1^{(3,2)}/g$	$\Omega_2^{(3,2)}/g$
-0.00	11.952987	4.015733	15.958206	8.020952	19.973939	4.005219
-0.10	11.955678	4.006464	15.961996	8.012782	19.974723	4.000055
-0.25	11.957932	3.993165	15.966096	8.001330	19.974919	3.992507
-0.50	11.956946	3.972586	15.968719	7.984360	19.972632	3.980447
-1.00	11.937254	3.937254	15.958261	7.958261	19.958261	3.958261
-2.00	11.826744	3.889490	15.874508	7.937254	19.890241	3.921521
-3.00	11.618950	3.872983	15.705143	7.959176	19.769413	3.894906
-4.00	11.307441	3.891243	15.444795	8.028595	19.594811	3.878578
-5.00	10.880300	3.952097	15.083052	8.154848	19.364917	3.872983
-6.00	10.316246	4.071248	14.600739	8.355741	19.077582	3.878898
-7.00	9.573955	4.282452	13.959460	8.667957	18.729907	3.897510
-8.00	8.550870	4.677887	13.060789	9.187806	18.318045	3.930550
-9.00	6.244998	6.244998	10.908712	10.908712	17.836915	3.980509
-11.00					16.637303	4.147307
-13.00					15.038297	4.455292
-15.00					12.817255	5.071289
-17.00					7.937254	7.937254

(38)

5 Local rf-pulses

Here we give two (ideal) local rf-pulse sequences needed to produce the true, canonical CNOT from the [CNOT] located in the Weyl chamber via

$$\text{CNOT} = e^{i\,\pi/4}\, k_1\, [\text{CNOT}]\, k_2. \tag{39}$$

Sequence 1: Total rotation $\varphi = 3\pi/2$,

$$k_1 = e^{-\frac{\pi}{2} Y_1}\, e^{\frac{\pi}{2}(X_1 - X_2)}, \quad k_2 = e^{\frac{\pi}{2} Y_1}. \tag{40}$$

Sequence 2: Total rotation $\varphi = 3\pi/2$,

$$k_1 = e^{-\frac{\pi}{2} Y_1}, \quad k_2 = e^{-\frac{\pi}{2} Z_1}\, e^{\frac{\pi}{2}(X_1 - X_2)}. \tag{41}$$

6 Fidelity degradation by switching to resonance

We are now going to consider the effect of switching — the actual process of bringing the qubits to resonance with external *rf*-field.

We will assume that [CNOT] generation is performed in three stages:

Stage 1. Tuning: Very fast linear rise of Rabi frequencies to their optimal values (for a given k), with time-dependent Hamiltonian

$$-\,iH_{\text{tune}} = -\left[\left(\Omega_1^{\text{opt}}\,X_1 + \Omega_2^{\text{opt}}\,X_2\right)\,\frac{t}{\epsilon\,t_{\text{gate}}} + g(XX+YY+kZZ)\right], \tag{42}$$

where $\epsilon \ll 1$ characterizes the fraction of the total gate time spent in the switching mode (tune/detune). We denote the corresponding time evolution by U_{tune};

Stage 2. Resonance: Evolution with optimal Rabi frequencies for most part of [CNOT] generation, $U_{\text{resonance}}$, where

$$\begin{aligned} U_{\text{resonance}} &= e^{-i\,(1-2\,\epsilon)\,t_{\text{gate}}\,H_{\text{resonance}}}, \\ -iH_{\text{resonance}} &= -\left[\Omega_1^{\text{opt}}\,X_1 + \Omega_2^{\text{opt}}\,X_2 + g(XX+YY+kZZ)\right], \end{aligned} \tag{43}$$

and

Stage 3. Detuning: Fast linear decrease of Rabi frequencies to zero, with time-dependent Hamiltonian

$$-\,iH_{\text{detune}} = -\left[\left(\Omega_1^{\text{opt}}\,X_1 + \Omega_2^{\text{opt}}\,X_2\right)\left(1-\frac{t}{\epsilon\,t_{\text{gate}}}\right) + g(XX+YY+kZZ)\right]. \tag{44}$$

The full gate is then the product

$$[\text{CNOT}]_{\text{opt}} = U_{\text{detune}}U_{\text{resonance}}U_{\text{tune}}. \tag{45}$$

In order to find the optimal values of the gate parameters, we first truncate the Magnus expansion for each switching part of the gate:

$$U_{\text{switching}}\,(\epsilon\,t_{\text{gate}}) = e^{\sigma(\epsilon\,t_{\text{gate}})}, \tag{46}$$

with

$$\begin{aligned} \sigma\,(\epsilon\,t_{\text{gate}}) \;\approx\; & -i\int_0^{\epsilon\,t_{\text{gate}}} dt H_{\text{switching}}(t) \\ & + \frac{(-i)^2}{2}\int_0^{\epsilon\,t_{\text{gate}}} dt_1\left[H_{\text{switching}}(t_1),\, \int_0^{t_1} dt_2\,H_{\text{switching}}(t_2)\right], \end{aligned} \tag{47}$$

and then use the 4th order iteration method [13]

$$\begin{aligned} U_{n+1} &= e^{\sigma_n}\,U_n, \\ \sigma_n &= \frac{h}{2}\,(A_1+A_2) + \frac{\sqrt{3}\,h^2}{12}\,[A_1,\,A_2], \\ A_1 &= -iH_{\text{switching}}(t_n + c_1 h), \\ A_2 &= -iH_{\text{switching}}(t_n + c_2 h), \\ h &= \frac{\epsilon\,t_{\text{gate}}}{N}, \end{aligned} \tag{48}$$

where N is the number of iteration steps and

$$c_{1,2} = \frac{1}{2} \pm \frac{\sqrt{6}}{3} \tag{49}$$

are the nodes of the Gauss-Legendre 4th order quadrature in [0, 1]. As described in [13], despite the presence of only h and h^2 terms, this is indeed the 4th order approximation to the Magnus expansion.

Optimization of gate's parameters was performed using Nelder-Mead simplex direct search with bound constraints [14] for the minimum of the square of the Frobenius distance

$$d^2_{\text{Frobenius}} = \operatorname{tr}\left[\left([\text{CNOT}] - [\text{CNOT}]_{\text{opt}}\right)^\dagger \left([\text{CNOT}] - [\text{CNOT}]_{\text{opt}}\right)\right] \tag{50}$$

between the optimal $[\text{CNOT}]_{\text{opt}}$ given by (45) and the perfect [CNOT] given in (23). Due to the enormous richness of possible CNOTs, we optimized only the most interesting of them. With $N = 2500$ we simulated the switching mechanism for $\epsilon = 0.025$:

k	Ω_1^{opt}/g	Ω_2^{opt}/g	$t_{\text{gate}}, \times\pi/(2g)$	$d^2_{\text{Frobenius}}, \times 10^{-3}$
0.50	8.130446	0.064667	0.999268	1.9
0.25	8.141971	0.032287	0.999363	1.6
0.10	8.145193	0.012910	0.999390	1.5
0.00	8.145807	0.000000	0.999395	1.5
−0.10	12.269887	4.111716	0.999382	1.5
−0.25	12.272602	4.098223	0.999348	1.6
−0.50	12.272970	4.077597	0.999237	1.9

(51)

Using the local pulses given in Section 5 we can transform the corresponding optimal $[\text{CNOT}]_{\text{opt}}$ to its canonical form. For example,

$$\text{CNOT}_{k=0.25} = \begin{bmatrix} 0.9998 - 0.0025i & -0.0001 - 0.0017i & -0.0001 - 0.0047i & 0.0192i \\ -0.0001 - 0.0017i & 0.9998 - 0.0025i & -0.0193i & 0.0001 + 0.0047i \\ 0.0193i & 0.0047i & 0.0001 - 0.0007i & 0.9998 + 0.0025i \\ -0.0001 - 0.0047i & -0.0192i & 0.9998 + 0.0025i & 0.0001 - 0.0007i \end{bmatrix}, \tag{52}$$

whose intrinsic fidelity relative to the computational basis is

$$F = \frac{1}{4}\sum_{r=1}^{4} \left|\left(\text{CNOT}^\dagger \cdot \text{CNOT}_{k=0.25}\right)_{rr}\right| = 0.9998. \tag{53}$$

7 Conclusion

To recapitulate, we have demonstrated how to implement various high-fidelity, plug-and-play CNOT logic gates by a single application of Hamiltonians used to describe coupled superconducting qubits. Architectures involving capacitive and inductive couplings have been analyzed for which the physical parameters required to generate the perfect CNOT have been found in closed, analytic form. Additional numerical simulations based on 4th order Magnus expansion were used to correct this ideal limit by taking into account the switching to resonance.

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Appendix: Derivation of the Hamiltonian for inductively coupled flux qubits

The system consists of two superconducting loops of self-inductance L coupled by a mutual inductance M and driven by external magnetic fluxes Φ_i, as shown on Fig. 1. Each loop is interrupted by a Josephson junction of critical current I_0 and effective capacitance C.

Inside the superconducting material, the Ginzburg-Landau complex order parameter can be written in the usual form,

$$\psi(\mathbf{r}) = \sqrt{\rho_{\rm s}(\mathbf{r})}e^{i\theta(\mathbf{r})}, \tag{A-1}$$

where $\rho_{\rm s}$ is the density of Cooper pairs. The supercurrent flux is

$$\mathbf{j}_{\rm s} = \frac{\hbar\rho_{\rm s}}{m^*}\left(\nabla\theta - \frac{q}{\hbar}\mathbf{A}_{\rm s}\right), \tag{A-2}$$

where $\mathbf{A}_{\rm s}$ is the vector potential inside the superconductor and $q = -2e$. The gauge is assumed to be chosen in such a way as to guarantee $\hat{\mathbf{n}}\cdot\mathbf{j}_{\rm s} = \mathbf{0}$ at the surface. In the clean limit, $\mathbf{j}_{\rm s} = \mathbf{0}$ inside the material, which leads to

$$\mathbf{A}_{\rm s} = \frac{\hbar}{q}\nabla\theta. \tag{A-3}$$

The line integral of $\mathbf{A}$ around Loop 1 is (here, the limits of integration 1 and 2 denote the two sides of the junction, the rest of notation is clear from context):

$$\begin{aligned}
\oint_{\text{Loop 1}} \mathbf{A}d\mathbf{l} &= \left(\int_1^2 \mathbf{A}d\mathbf{l}\right)_{\text{inside JJ}} + \left(\int_2^1 \mathbf{A}d\mathbf{l}\right)_{\text{in the rest of circuit (inside superconducting bulk)}} \\
&= \left[\int_1^2 \mathbf{A}_{\rm JJ}d\mathbf{l} - \frac{\hbar}{q}(\theta_2-\theta_1)\right] + \left[\frac{\hbar}{q}(\theta_2-\theta_1) - \int_1^2 \mathbf{A}_{\rm s}d\mathbf{l}\right] \\
&= -\frac{\hbar}{q}\left[(\theta_2-\theta_1) - \frac{q}{\hbar}\int_1^2 \mathbf{A}_{\rm JJ}d\mathbf{l}\right] - \frac{\hbar}{q}\left[(\theta_1-\theta_2) + \int_1^2 \nabla\theta d\mathbf{l}\right] \\
&= -\frac{\hbar}{q}\left[\phi_1 + \oint_{\text{Loop 1}} \nabla\theta d\mathbf{l}\right] \\
&= -\frac{\hbar}{q}(\phi_1 + 2\pi n_1),
\end{aligned} \tag{A-4}$$

where ϕ_1 is the gauge invariant phase difference across the first junction, and $n_1 = 0, 1, 2, 3, \ldots$. This "quantization" condition is justified by the fact that the order parameter is nonzero inside the junction [15]. Alternatively,

$$\oint_{\text{Loop 1}} \mathbf{A}d\mathbf{l} = \Phi_1^{\text{external}} + \Phi_1^{\text{self}} + \Phi_1^{\text{mutual}} = \Phi_1 - LI_1 + MI_2. \tag{A-5}$$

Introducing

$$\alpha = \frac{\hbar}{2e} = \frac{\Phi_{\rm sc}}{2\pi}, \quad E_J = \alpha I_0, \quad \omega_0 = \frac{1}{\sqrt{LC}}, \quad E_0 = \frac{\alpha^2}{L} = \frac{\hbar^2\omega_0^2}{2E_C}, \quad E_C = \frac{(2e)^2}{2C}, \quad \Upsilon = \frac{M}{L}, \tag{A-6}$$

and taking into account (A-4) and (A-5) together with the Josephson equations, we get the equations of motion for the two gauge-invariant phase differences,

$$\begin{aligned}
\alpha^2 C\left(\ddot{\phi}_1 - \Upsilon\ddot{\phi}_2\right) &= -E_J\left(\sin\phi_1 - \Upsilon\sin\phi_2\right) - E_0\left(\phi_1 + 2\pi n_1 - \frac{2\pi\Phi_1}{\Phi_{\rm sc}}\right), \\
\alpha^2 C\left(\ddot{\phi}_2 - \Upsilon\ddot{\phi}_1\right) &= -E_J\left(\sin\phi_2 - \Upsilon\sin\phi_1\right) - E_0\left(\phi_2 + 2\pi n_2 - \frac{2\pi\Phi_2}{\Phi_{\rm sc}}\right).
\end{aligned} \tag{A-7}$$

It is clear that $2\pi n_i$ are not dynamical and can be absorbed into $\phi_i + 2\pi n_i \to \phi_i$ without affecting any physics. Notice also that in the limit $M \to 0$ we correctly recover a well-known result for two independent loops.

Because of the presence of terms $\Upsilon E_J \sin\phi_i$ in (A-7), we cannot immediately deduce system's Lagrangian. However, by multiplying the second equation in (A-7) by Υ, and by adding the result to the first equation, we can separate the variables

$$\alpha^2 C\left(1-\Upsilon^2\right)\ddot{\phi}_1 = -E_J\left(1-\Upsilon^2\right)\sin\phi_1 - E_0\left[\left(\phi_1 - \frac{2\pi\Phi_1}{\Phi_{\rm sc}}\right) + \Upsilon\left(\phi_2 - \frac{2\pi\Phi_2}{\Phi_{\rm sc}}\right)\right], \tag{A-8}$$

and similarly for $\ddot{\phi}_2$. The Lagrangian is now easily found to be

$$\begin{aligned}
L &= \left(1-\Upsilon^2\right)\left\{\frac{\alpha^2 C}{2}\left(\dot{\phi}_1^{\,2} + \dot{\phi}_2^{\,2}\right) + E_J(\cos\phi_1 + \cos\phi_2)\right\} \\
&\qquad - \frac{E_0}{2}\left[\left(\phi_1 - \frac{2\pi\Phi_1}{\Phi_{\rm sc}}\right)^2 + \left(\phi_2 - \frac{2\pi\Phi_2}{\Phi_{\rm sc}}\right)^2\right] \\
&\qquad - \Upsilon E_0\left(\phi_1 - \frac{2\pi\Phi_1}{\Phi_{\rm sc}}\right)\left(\phi_2 - \frac{2\pi\Phi_2}{\Phi_{\rm sc}}\right).
\end{aligned} \tag{A-9}$$

In the limit of weak coupling ($\Upsilon \ll 1$) the terms $\sim \Upsilon^2$ can be dropped, giving

$$H = \frac{p_1^2 + p_2^2}{2m} + U(\phi_1, \phi_2), \tag{A-10}$$

with $p_i = m\dot{\phi}_i$, $m = \alpha^2 C$, and

$$U(\phi_1,\phi_2) = \sum_{i=1}^{2}\left[-E_J\cos\phi_i + \frac{E_0}{2}\left(\phi_i - \frac{2\pi\Phi_i}{\Phi_{\rm sc}}\right)^2\right] + \Upsilon E_0\left(\phi_1 - \frac{2\pi\Phi_1}{\Phi_{\rm sc}}\right)\left(\phi_2 - \frac{2\pi\Phi_2}{\Phi_{\rm sc}}\right). \tag{A-11}$$

After projecting onto the qubit subspace and using RWA we recover (13).

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